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17698 U.S. PTO  
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## PROVISIONAL APPLICATION FOR PATENT COVER SHEET

This is a request for filing a PROVISIONAL APPLICATION FOR PATENT under 37 CFR 1.53(c).

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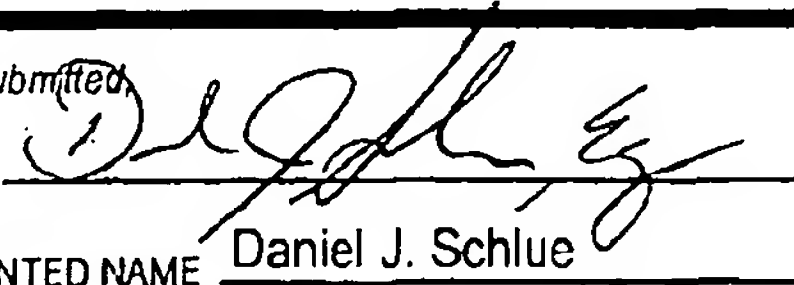
INVENTOR(S)					
Given Name (first and middle (if any))		Family Name or Surname		Residence (City and either State or Foreign Country)	
Jun		Hu		Fairlawn, OH	
<input type="checkbox"/> Additional inventors are being named on the _____ separately numbered sheets attached hereto					
TITLE OF THE INVENTION (500 characters max)					
7-ETHYNYL-2,4,9-TRITHIAADAMANTANE AND RELATED METHODS					
Direct all correspondence to: CORRESPONDENCE ADDRESS					
<input type="checkbox"/> Customer Number		<input type="text"/>		<input type="checkbox"/> Place Customer Number Bar Code Label here	
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Address					
City	Akron	State	Ohio	ZIP	44308
Country	US	Telephone	330-849-6777	Fax	330-376-4577
ENCLOSED APPLICATION PARTS (check all that apply)					
<input checked="" type="checkbox"/> Specification	Number of Pages	23	<input type="checkbox"/> CD(s), Number	<input type="text"/>	
<input checked="" type="checkbox"/> Drawing(s)	Number of Sheets	4	<input type="checkbox"/> Other (specify)	<input type="text"/>	
<input type="checkbox"/> Application Data Sheet. See 37 CFR 1.76					
METHOD OF PAYMENT OF FILING FEES FOR THIS PROVISIONAL APPLICATION FOR PATENT					
<input checked="" type="checkbox"/>	Applicant claims small entity status. See 37 CFR 1.27.			FILING FEE AMOUNT (\$)	
<input type="checkbox"/>	A check or money order is enclosed to cover the filing fees				
<input checked="" type="checkbox"/>	The Commissioner is hereby authorized to charge filing fees or credit any overpayment to Deposit Account Number: 50-0959(089498-0467)			\$80.00	
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The invention was made by an agency of the United States Government or under a contract with an agency of the United States Government.					
<input checked="" type="checkbox"/>	No.				
<input type="checkbox"/>	Yes, the name of the U.S. Government agency and the Government contract number are: _____				

Respectfully submitted

SIGNATURE

TYPED or PRINTED NAME

TELEPHONE

  
Daniel J. Schlue

330-849-6777

Date

07/01/2003

REGISTRATION NO.

(if appropriate)

Docket Number:

52,194

089498-0467

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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In the application of

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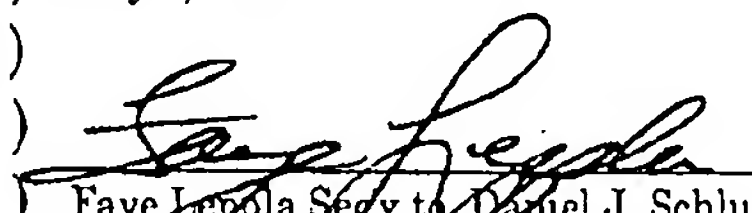
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For 7-ETHYNYL-2,4,9-TRITHIAADAMANTANE  
AND RELATED METHODS

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TRANSMITTAL SHEET

Enclosed are the following documents:

Provisional Application Cover Sheet

Provisional Patent Application

4 Sheets of Drawings (Figs. 1-4)

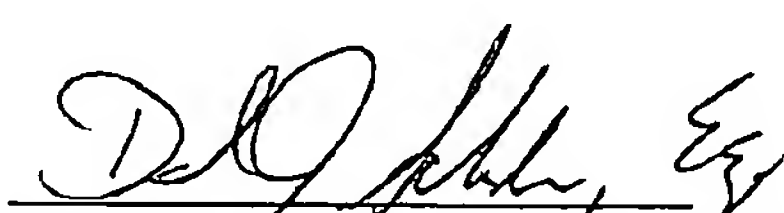
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Respectfully submitted

  
Daniel J. Schlue, Reg. No. 52,194  
Roetzel & Andress  
222 Main St.  
Akron, Ohio 44308  
(330) 849-6777  
Attorney for Applicant

July 1, 2003

## 7-ETHYNYL-2,4,9-TRITHIAADAMANTANE AND RELATED METHODS

5

### TECHNICAL FIELD

This invention relates to 7-ethynyl-2,4,9-trithiaadamantane, a method for its manufacture, and molecular wires having at least one trithiaadamantane surface anchor.

### BACKGROUND OF THE INVENTION

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In molecular-electronics manufacturing, there is a long-standing need to integrate or "anchor" a molecular wire into electronic circuitry. Molecular wires are substances or compounds that can transmit a signal between two points in a circuit. The signal is usually electronic, but it can be mechanical, optical, or even magnetic. And when the signal is electronic, the wires are often described as organic molecules with conjugated electronic systems that can effectively transmit electrons one dimensionally.

15

A molecular wire has one or more chemical functionalities that can bond to a metallic surface- and this is what secures the wire to a surface. These chemical functionalities are commonly referred to as surface anchors. Anchors also act as the wire-electrode interface. So it's important that the anchor provide a stable interface that facilitates the transmission of a signal.

20

A molecular wire becomes a molecular device when it bonds, via a surface anchor, to at least one electrode of an electronic circuit. A diode is such a molecular device. Molecular devices are used to control current characteristics or quantum effects on current-voltage behavior.

25

Many conventional surface anchors have a single sulfur atom that chemically bonds with a subject metallic surface, i.e., surfaces of electronic circuitry. So when these types of sulfur-based anchors are employed, the target substrate is typically coated with a thin gold film because a relatively strong bond forms between sulfur and gold. And although single sulphur-metal bonds do form, prior-art anchors based on single thiols or thioethers are inadequate because of: (1) the chemical instability that results from only a single bond with a target substrate and (2) the resulting surface orientation is unpredictable.

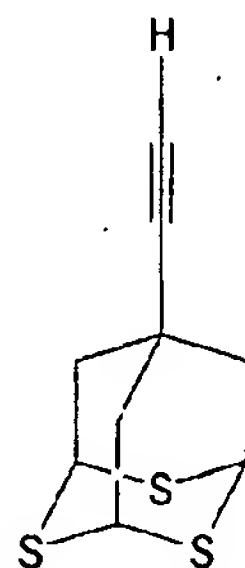
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More specifically regarding surface orientation, anchors that form only a single sulfur-metal bond with a metallic surface have a surface orientation that is often uncontrollable and unpredictable. For example, such an anchor's surface orientation could be either substantially vertical or substantially parallel to a metallic-film surface. Unpredictable surface orientation is problematic because it directly impacts the spatial orientation of the entire molecular wire.

The art can therefore be improved by providing anchors with improved stability and more predictable surface orientation compared to prior-art single-sulfur anchors. More specifically, the art can be improved with anchors that form multiple sulfur-metal bonds.

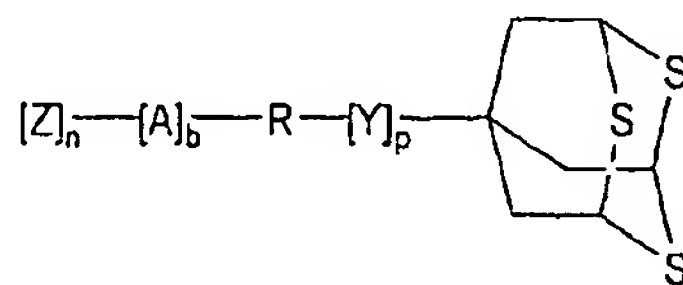
### SUMMARY OF THE INVENTION

This invention provides a compound having the formula:



This invention further provides a method for manufacturing 7-ethynyl-2,4,9-trithiaadamantane comprising the step of: reacting 7-carbonyl-2,4,9-trithiaadamantane with Ohira-Bestmann reagent to produce 7-ethynyl-2,4,9-trithiaadamantane.

Also provided is a molecular wire having the formula:



wherein A and Y are independently selected chemical functionalities,

wherein p is 0 or 1,

wherein b is 0 or an integer greater than or equal to 1,

wherein R is a compound that is capable of transferring a signal,

wherein Z is a surface anchor, and

wherein n is 0 or an integer greater than or equal to 1.

Also provided is a method for manufacturing a molecular wire comprising the step of chemically bonding, either directly or indirectly, trithiaadamantane to a compound that is capable of transferring a signal.

Also provided is a method for manufacturing 7-ethynyl-2,4,9-trithiaadamantane comprising the step of: reducing an alkyl 2,4,9-trithiaadamantane-7-carboxylate to produce 7-hydroxymethyl-2,4,9-trithiaadamantane; and oxidizing 7-hydroxymethyl-2,4,9-trithiaadamantane to produce 7-carbonyl-2,4,9-trithiaadamantane.

#### BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 is a polarization modulation FT-IR reflectance absorption of a self-assembled monolayer of 7-ethynyl-2,4,9-trithiaadamantane on a thin gold film.

Fig. 2 is a self-assembled monolayer of 7-ethynyl-2,4,9-trithiaadamantane on colloidal gold nanoparticles observed by UV-vis Absorption.

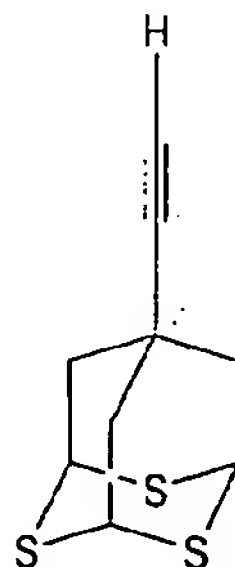
Fig. 3 is an X-ray crystal structure of a Cu(II)-linked molecular wire.

Fig. 4 is an X-ray crystal structure of 7-ethynyl-2,4,9-trithiaadamantane.

#### DETAILED DESCRIPTION OF THE ILLUSTRATIVE EMBODIMENTS

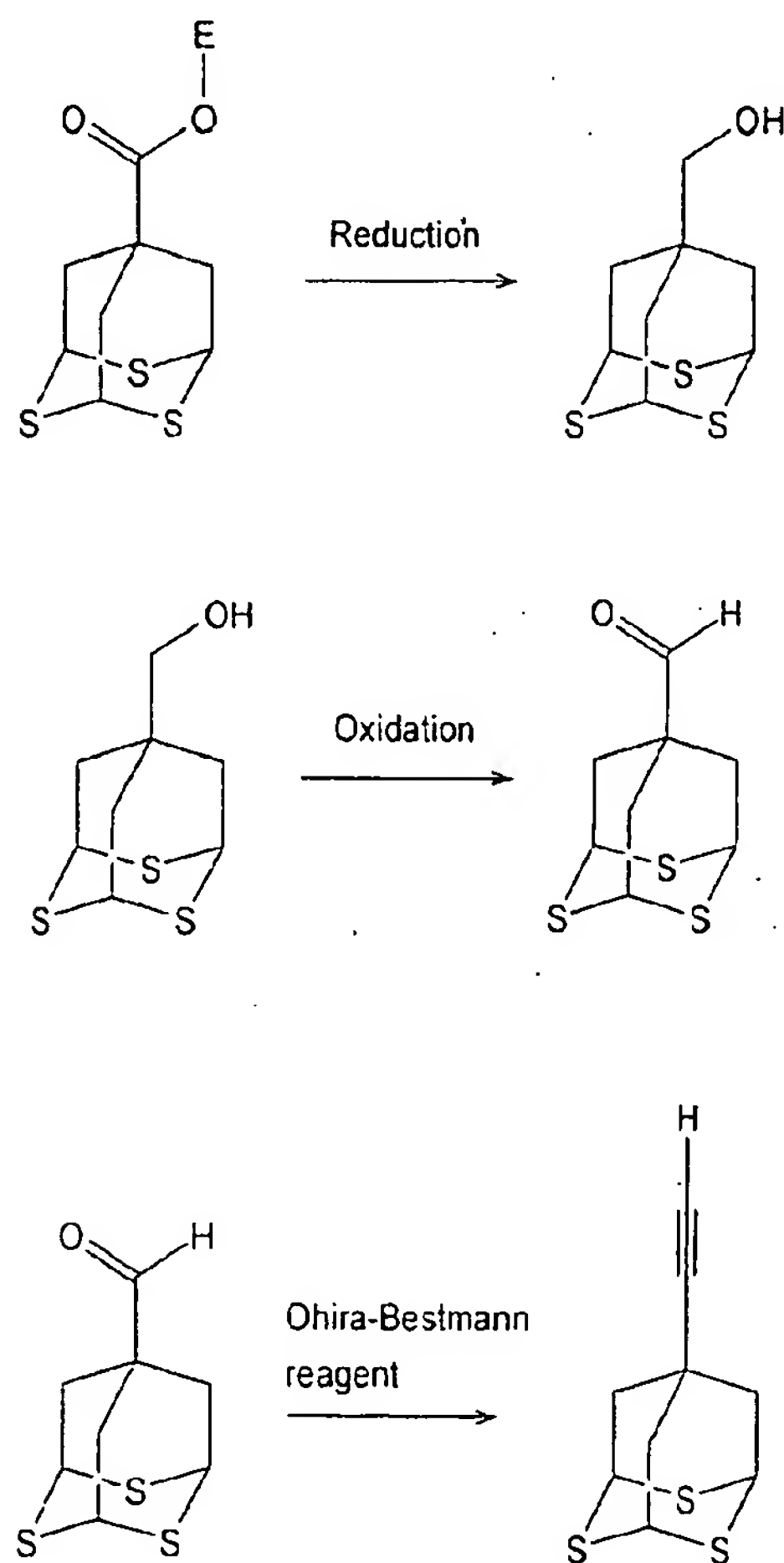
This invention is generally directed to 7-ethynyl-2,4,9-trithiaadamantane, a method for its manufacture, and molecular wires having at least one trithiaadamantane surface anchor.

7-ethynyl-2,4,9-trithiaadamantane is represented by the formula:



7-ethynyl-2,4,9-trithiaadamantane can be manufactured in three steps. First, an alkyl 2,4,9-trithiaadamantane-7-carboxylate is reduced to produce 7-hydroxymethyl-2,4,9-trithiaadamantane. Second, 7-hydroxymethyl-2,4,9-trithiaadamantane is oxidized to produce 7-carbonyl-2,4,9-trithiaadamantane. Third, 7-carbonyl-2,4,9-trithiaadamantane is reacted with Ohira-Bestmann reagent to produce 7-ethynyl-2,4,9-trithiaadamantane.

The method for manufacturing 7-ethynyl-2,4,9-trithiaadamantane is represented by the simplified reaction scheme:

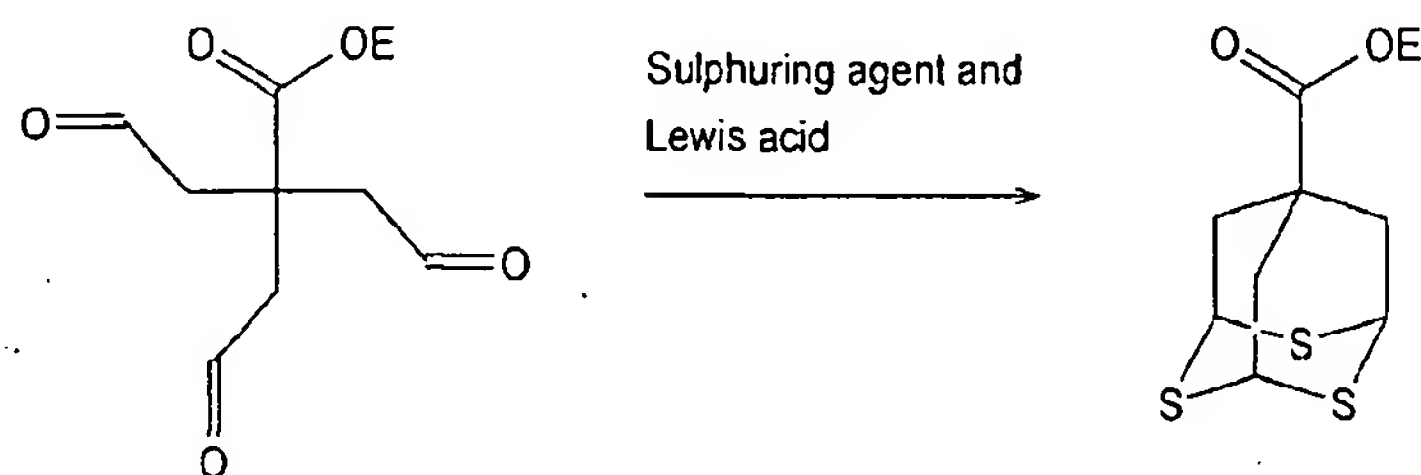




**METHOD****First Step**

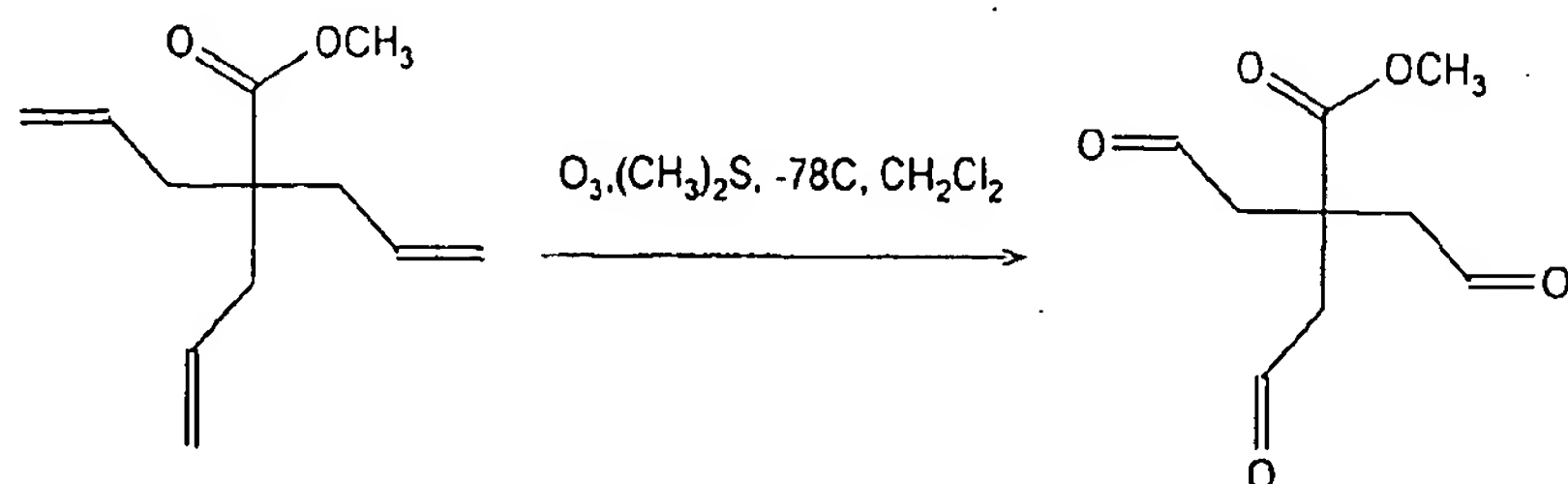
In performing the first step, an alkyl 2,4,9-trithiaadamantane-7-carboxylate is  
 5 reduced to produce 7-hydroxymethyl-2,4,9-trithiaadamantane. There are no limitations on  
 the type of alkyl group that can be employed in the reaction, but a methyl group is  
 preferred.

Alkyl 2,4,9-trithiaadamantane-7-carboxylate can be synthesized by reacting an  
 oxidized alkyl triallyl acetate with a sulphuring agent and a Lewis acid. A general  
 10 understanding of which can be gained from the following simplified reaction scheme:



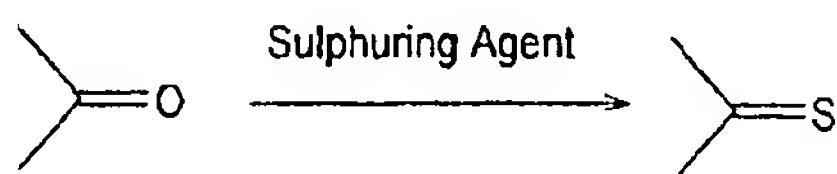
wherein E is an alkyl.

Oxidized alkyl triallyl acetate is manufactured by simply oxidizing an alkyl  
 triallyl acetate. Any method of oxidation can be employed, but ozonolysis is preferred. An  
 15 example of oxidizing methyl triallyl acetate via ozonolysis uses a solution of methyl triallyl  
 acetate in freshly-distilled methylenechloride followed by stirring and cooling the solution  
 to  $-78^{\circ}\text{C}$  in a dry-ice acetone bath. Ozone is subsequently bubbled through the cooled  
 solution until a light-blue color persists. This method for oxidation is generally represented  
 by the reaction scheme:



Any useful sulphuring agent can be employed in synthesizing an alkyl 2,4,9-trithiaadamantane-7-carboxylate. A sulfuring agent converts ketonic groups into thioketonic groups as represented by the reaction scheme:

5



10

Preferred sulphuring agents include 1,3,2,4-dithiadiphosphetane-2,4-disulfide (Lawesson's reagent), phosphorous pentasulfide hexamethyldisiloxane (PPHD), or combinations thereof.

The relative mole ratio of sulphuring agent to oxidized alkyl triallyl acetate can generally range from about 6:1 to about 1:1. Preferably, the mole ratio ranges from about 3:1 to about 2:1.

15

Any Lewis acid can be employed in synthesizing an alkyl 2,4,9-trithiaadamantane-7-carboxylate. Preferred Lewis acids include the complex of boron trifluoride and ethyl ether ( $\text{BF}_3 \cdot \text{Et}_2\text{O}$ ), the complex of boron trichloride and ethyl ether ( $\text{BCl}_3 \cdot \text{Et}_2\text{O}$ ), or combinations thereof.

20

The mole ratio of Lewis acid to oxidized alkyl triallyl acetate preferably ranges from about 4:1 to about 1:1. More preferably, the mole ratio ranges from about 3:1 to about 2:1. Generally, the concentration of Lewis acid in the reaction medium ranges from about 0.5 to about 1.0 molar ( $M$ ).

25

In synthesizing an alkyl 2,4,9-trithiaadamantane-7-carboxylate, any noncoordinated or weakly coordinated reaction solvent can be employed. Nonlimiting examples of preferred solvents are methylene chloride ( $\text{CH}_2\text{Cl}_2$ ), carbon tetrachloride ( $\text{CCl}_4$ ), benzene, or combinations thereof. Effective amounts of noncoordinated or weakly coordinated solvent can be determined by a person of ordinary skill in the art without undue experimentation.

Synthesis of alkyl 2,4,9-trithiaadamantane-7-carboxylate preferably occurs under reflux, and a person of ordinary skill in the art can determine the temperatures required for reflux without undue experimentation.

Alkyl 2,4,9-trithiaadamantane-7-carboxylate can be reduced by any useful method. Preferably, alkyl 2,4,9-trithiaadamantane-7-carboxylate is initially reacted with a reducing agent followed by a subsequent reaction with a proton donor. Without being bound to theory, reaction between alkyl 2,4,9-trithiaadamantane-7-carboxylate and a reducing agent produces a salt, and the proton donor subsequently aids in disassociating the salt to produce 7-hydroxymethyl-2,4,9-trithiaadamantane.

Useful reducing agents are in no way limited. Preferred reducing agents include diisobutylaluminum hydride, sodium tetrahydridoborate, lithium aluminum hydride, or combinations thereof.

In a preferred embodiment for reducing alkyl 2,4,9-trithiaadamantane-7-carboxylate, the reducing agent is reacted with alkyl 2,4,9-trithiaadamantane-7-carboxylate in a relative mole ratio ranging from about 5:1 to about 1:1. Preferably, the relative mole ratio ranges from about 3:1 to about 1:1.

Any proton donor can be employed, and preferred proton donors include water, methanol, and ethanol. Relative to the alkyl 2,4,9-trithiaadamantane-7-carboxylate salt, an excess of proton donors are generally present in the reaction medium. Preferably, the proton donors are present at a relative mole ratio to alkyl 2,4,9-trithiaadamantane-7-carboxylate salt ranging from about 10:1 to about 1:1; more preferably from about 5:1 to about 1:1.

Reduction via the disclosed method is preferably conducted in a liquid reaction medium that is preferably an inert organic solvent. Useful inert organic solvents are not limited and include toluene, benzene, and combinations thereof.

And reduction preferably occurs at a temperature ranging from about -78 to about 35°C; preferably at temperatures ranging from about -10 to about 5°C. More preferably, reduction occurs at about 0°C.

### Second Step

The second step of the subject method oxidizes 7-hydroxymethyl-2,4,9-trithiaadamantane to produce 2,4,9-trithia-tricyclo[3.3.1.1<sup>3,7</sup>]dec-7-carbaldehyde. Oxidation is not limited to a particular method, although Swern oxidation conditions are preferred. Swern oxidation conditions are well known and generally describe a combination of reaction conditions such as reagents, temperature, pressure, and reaction medium. Preferred Swern oxidation conditions include at least one of the following three combinations of reagents: (1) oxalyl chloride and dimethyl sulfoxide; (2) trifluoroacetic anhydride and dimethylsulfoxide; and (3) triethylamine and diisopropylamine.

The Swern oxidation reagents are preferably present in an excess mole ratio relative to the amount of 7-hydroxymethyl-2,4,9-trithiaadamantane. In one embodiment, the Swern oxidation reagents are reacted with 7-hydroxymethyl-2,4,9-trithiaadamantane in a relative mole ratio ranging from about 5:1 to about 1:1, and in another embodiment, the relative mole ratio ranges from about 3:1 to about 1:1.

Oxidation is preferably conducted in an inert liquid reaction medium. Chlorinated organic solvents such as methylenechloride, carbontetrachloride, chloroform, and combinations thereof are preferred.

Oxidizing 7-hydroxymethyl-2,4,9-trithiaadamantane to produce (7-carbonyl-2,4,9-trithiaadamantane is preferably conducted under Swern oxidation conditions wherein the temperature ranges from about -100 to about -50°C. Preferably, the reaction is performed at a temperature of about -75°C.

### Third Step

The Ohira-Bestmann reagent is well known, and any form thereof can be employed in performing the third step of the subject method. A preferred Ohira-Bestmann reagent is at least one of  $\text{CH}_3\text{COC}(\text{N}_2)\text{P}(\text{O})(\text{OCH}_3)_2$  and  $\text{CH}_3\text{COC}(\text{N}_2)\text{P}(\text{O})(\text{OCH}_2\text{CH}_3)_2$  in combination with at least one of  $\text{K}_2\text{CO}_3$  and  $\text{Na}_2\text{CO}_3$ . So an example of a preferred Ohira-Bestmann reagent is the combination of  $\text{CH}_3\text{COC}(\text{N}_2)\text{P}(\text{O})(\text{OCH}_3)_2$  and  $\text{K}_2\text{CO}_3$ .

Generally, an excess of Ohira-Bestmann reagent is employed. Preferably, Ohira-Bestmann reagent is reacted with 7-carbonyl-2,4,9-trithiaadamantane in a relative



mole ratio ranging from about 5:1 to about 1:1, and more preferably from about 3:1 to about 1:1.

The third-step reaction between Ohira-Bestmann reagent and 7-carbonyl-2,4,9-trithiaadamantane is not limited to any particular reaction medium. Preferably, the reaction medium is an alcoholic solvent, and more preferably the reaction medium is selected from the group consisting of methanol and ethanol.

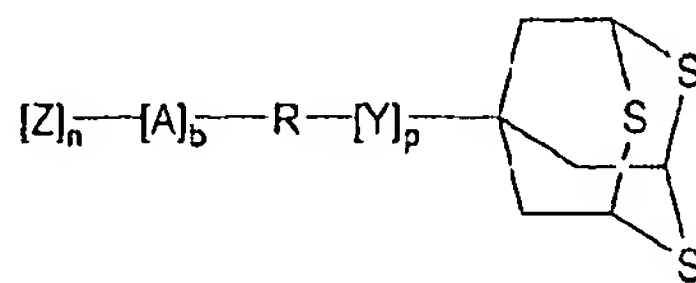
The third-step reaction is preferably conducted at a temperature ranging from about 20 to about 40°C. More preferably, the reaction is conducted at a temperature of about 30°C.

The subject method advantageously produces 7-ethynyl-2,4,9-trithiaadamantane at a yield greater than 50%. Preferably, the yield is greater than 75%.

#### Molecular Wire

The subject molecular wires have at least one trithiaadamantane surface anchor. The anchors are attached, either directly or indirectly, to a chemical compound that is capable of transmitting an electronic, optical, mechanical, or other type of signal. Indirect attachment occurs where a chemical functionality links the anchor to the compound. Any chemical functionality can be employed for indirect attachment, and preferred chemical functionalities include ethynyl and carboxylate. Direct attachment occurs where the anchor bonds with the compound, *i.e.*, no chemical functionality links the two together.

Useful molecular wires have the formula:



wherein A and Y are independently selected chemical functionalities,

wherein p is 0 or 1,

wherein b is 0 or an integer greater than or equal to 1,

wherein R is a compound that is capable of transferring a signal,

wherein Z is a surface anchor, and

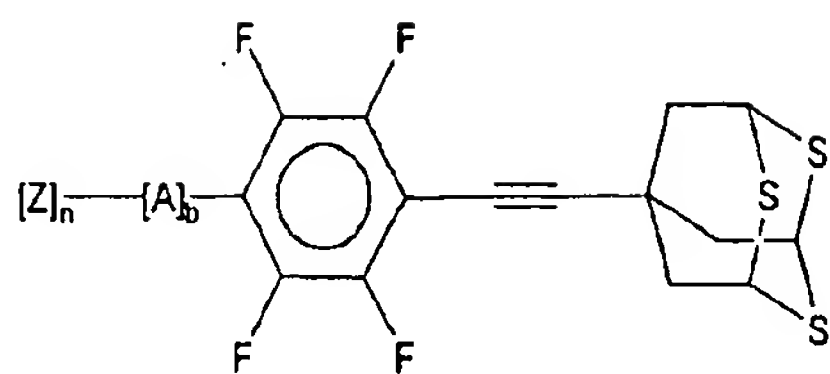
wherein  $n$  is 0 or an integer greater than or equal to 1.

When  $p$  is 0, trithiaadamantane is bonded directly to  $R$ . If  $b$  is 0 and  $n$  is an integer greater than or equal to 1, then  $R$  is bonded to directly to  $Z$ . Variables  $A$  and  $Y$  are preferably selected from ethynyl and carboxylate.

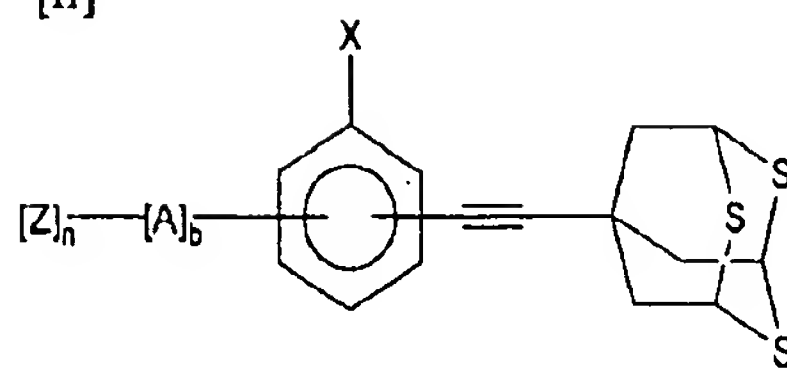
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The molecular wires are preferably selected from the following:

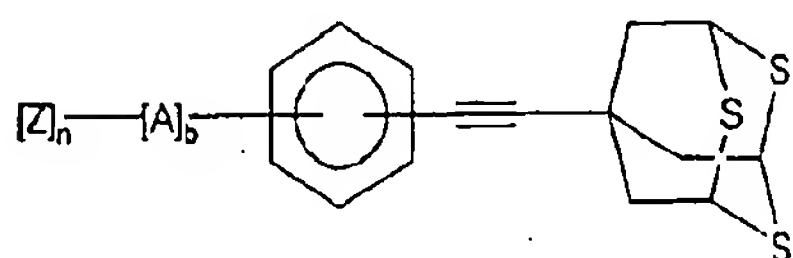
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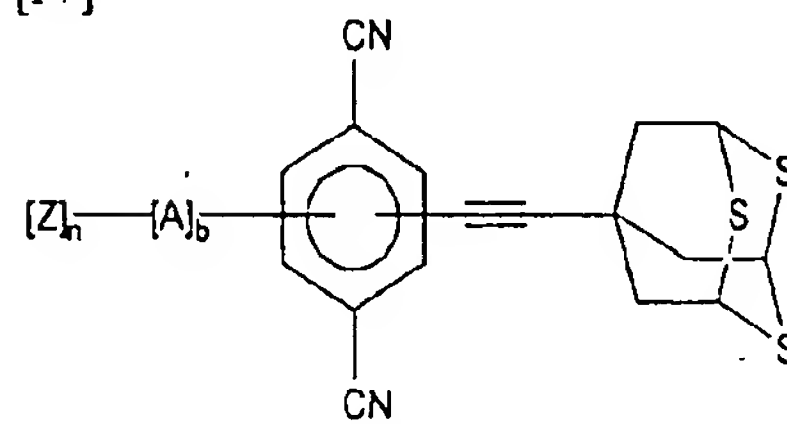
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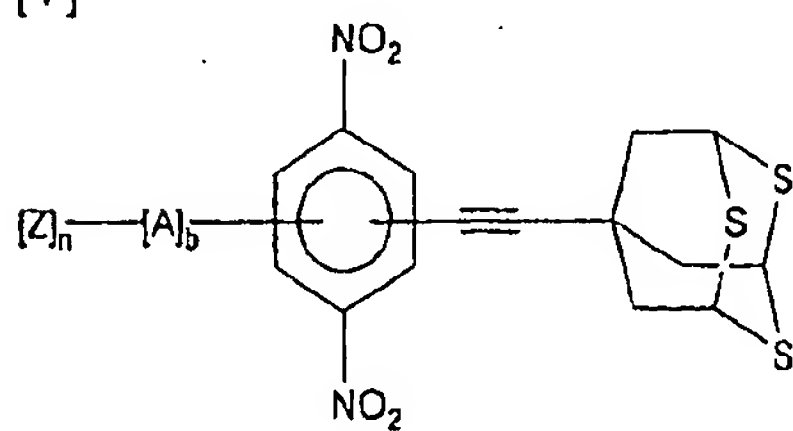
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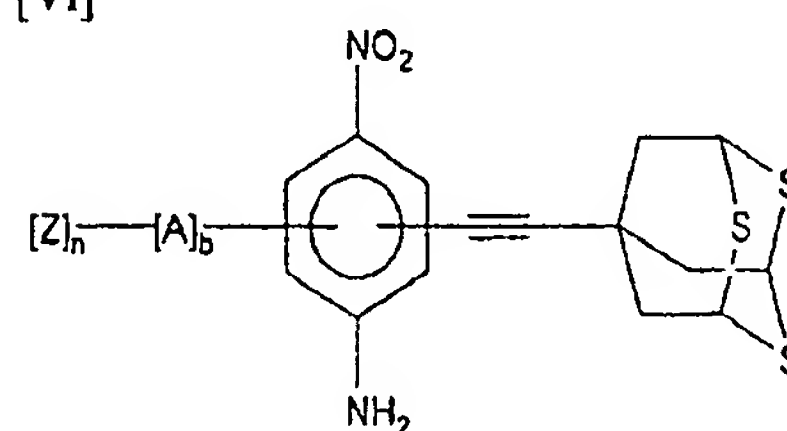
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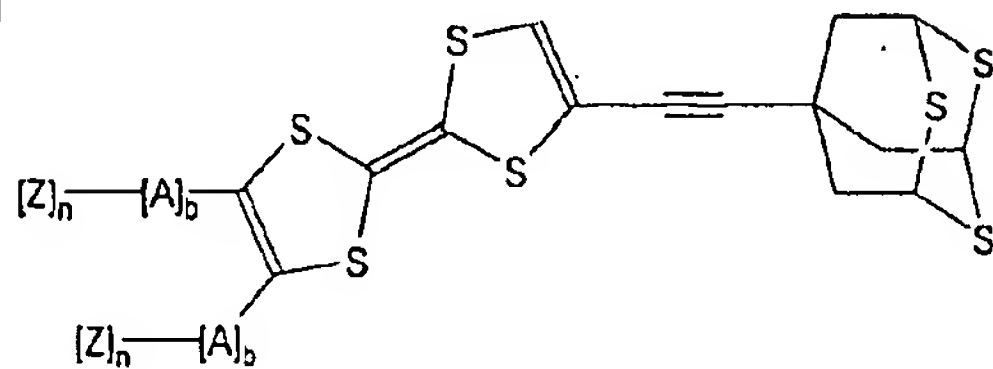
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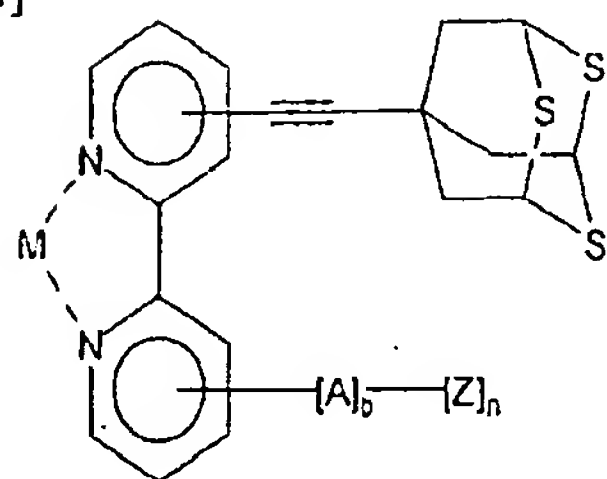
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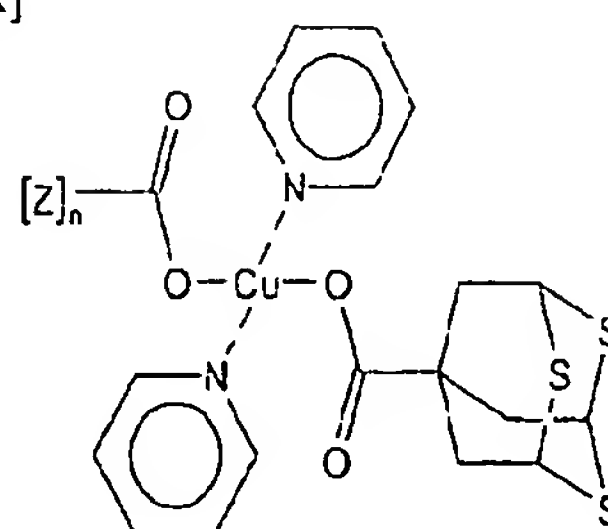
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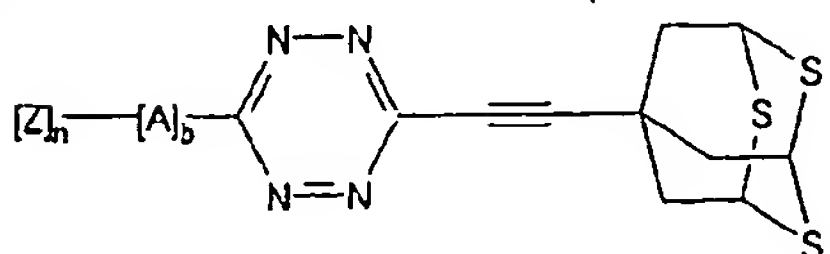
[VIII]



[IX]



[X]



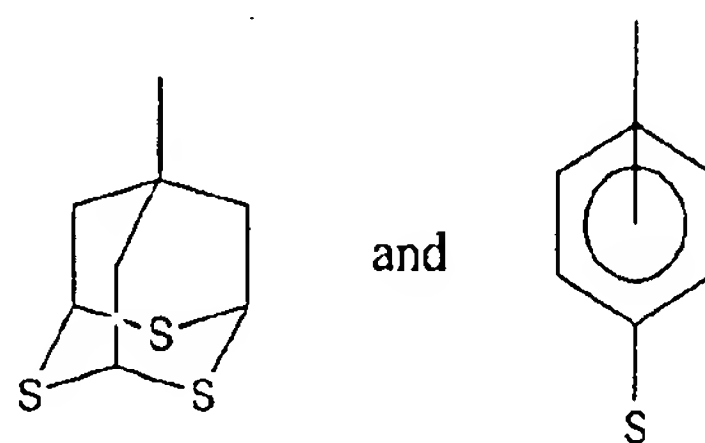
wherein M is a metallic element,  
wherein X is a halogen,  
wherein A, b, Z, and n are as described above.

5 Regarding the preferred molecular wires, trithiaadamantane, can bond, either directly or indirectly, with any available carbon atom on a cyclic organic compound- as indicated in the formulas by the loose position of the bond between trithiaadamantane and a cyclic compound. The same positional concept holds true for the variable Z, which is also depicted in the loose position.

10 The metallic element M, can be any metallic element, and it is preferably selected from platinum, palladium, or copper.

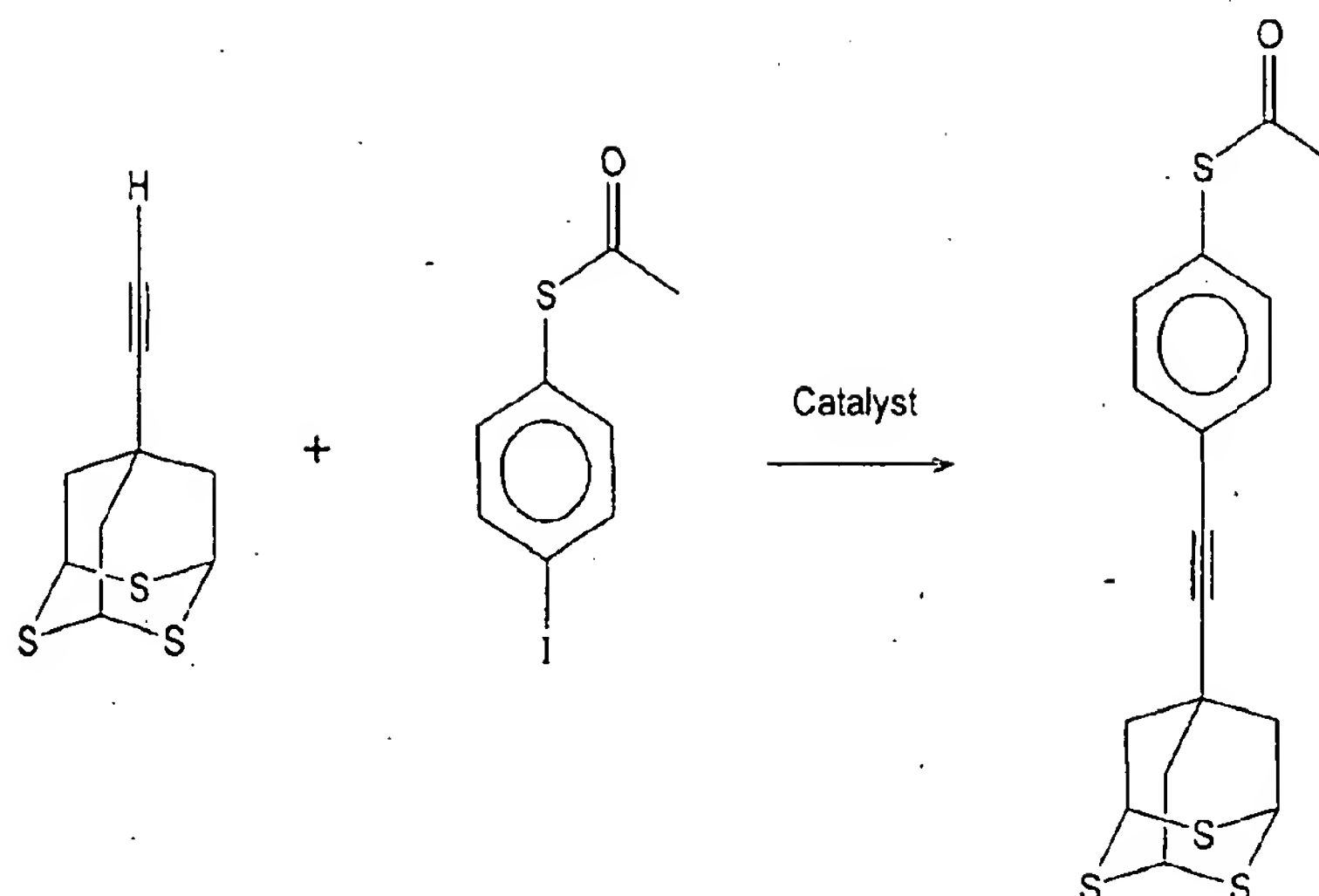
The halogen X is not limited to a specific halogen or group of halogens, but it is preferably fluorine, chlorine, bromine, or iodine.

15 The surface anchor Z can be any surface anchor, conventional or other, including trithiaadamantane. Nonlimiting examples of preferred surface anchors for the variable Z are:



20 The subject molecular wires can be made by using conventional chemical methods. For example, 7-ethynyl-2,4,9-trithiaadamantane can be cross coupled with 4-sulfur-acetylthioxy-iodobenzene by using the catalysts: CuI/diisopropylamine and Pd(PPh<sub>3</sub>)<sub>4</sub>. This synthesis is represented by the simplified reaction scheme:

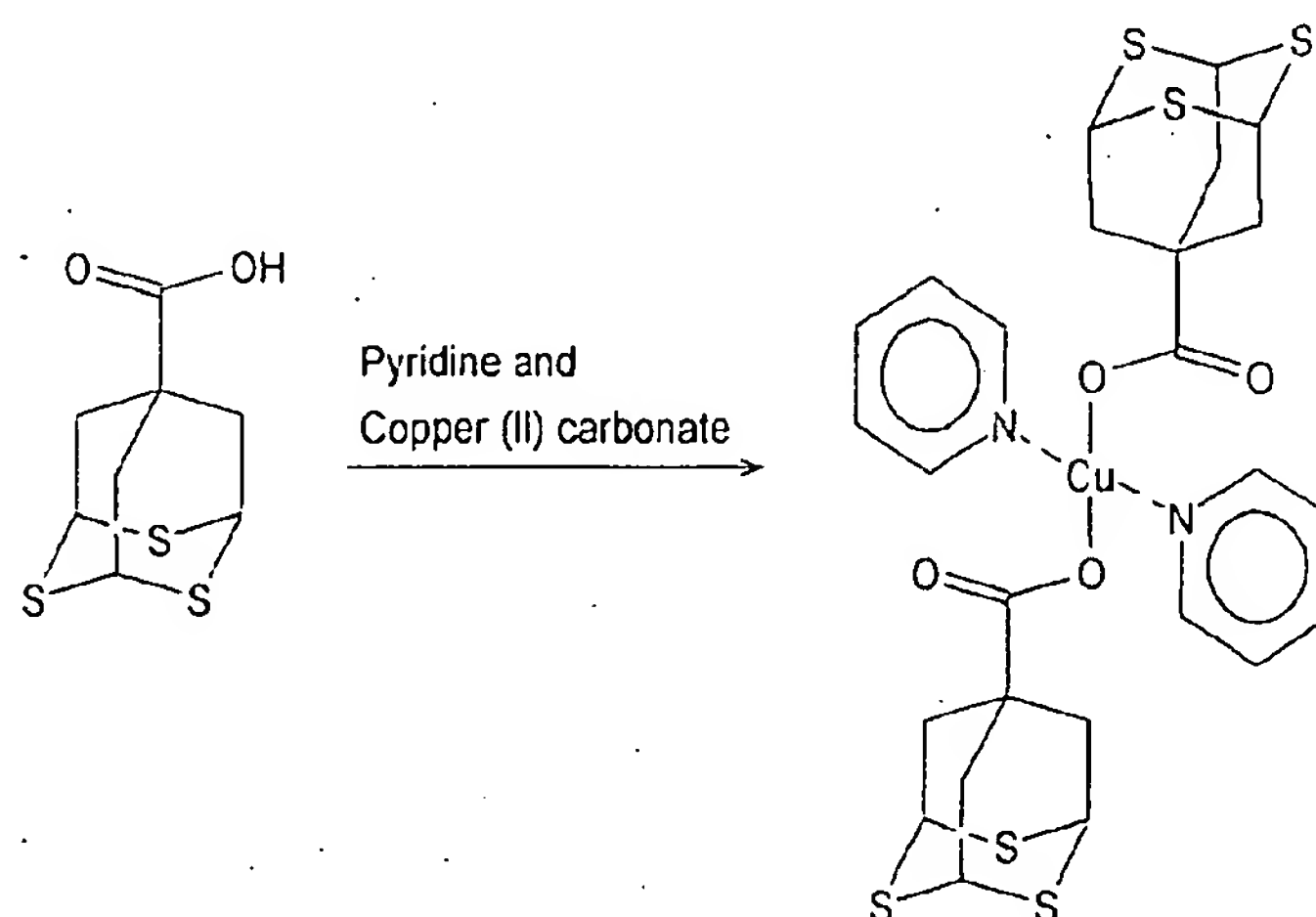




Reaction preferably occurs in an inert solvent such as dimethylformamide (DMF) and at a temperature ranging from about 75 to 150°C. More preferably, the reaction occurs under reflux for about two days.

5

An additional simplified reaction scheme for making a different molecular wire is presented:



The above reaction preferably occurs in pyridine and at a temperature ranging from about 20 to 50°C. Preferably, the reaction occurs at room temperature for about two days.

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## EXAMPLES

In order to demonstrate the present invention, the following examples have been prepared and tested. The examples should not, however, be viewed as limiting the scope of the invention. The claims will serve to define the invention.

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### *Methyl 7-hydroxycarbonyl-2,4,9-trithiaadamantane*

A solution of 5 grams of methyl triallyl acetate in 100 milliliters freshly distilled methylenechloride was stirred and cooled to  $-78^{\circ}\text{C}$  in a dry-ice acetone bath. Ozone was bubbled through the cooled mixture until a light-blue color persisted. The ozone  
10 line was then disconnected and the excess ozone was removed by argon flow for 10 minutes. 6.0 grams dimethyl sulfide was added to the reaction mixture at  $-78^{\circ}\text{C}$ . The mixture was slowly warmed up to the ambient temperature. The mixture was then concentrated via rotary evaporation. To this mixture, 100 milliliters of methylenechloride, 28.0 grams of Lawesson's reagent, and 100 milliliters of neat  $\text{BF}_3 \cdot \text{Et}_2\text{O}$  were added  
15 respectively. The mixture was then refluxed for 100 hours. Additional methylenechloride was added (100 mL). The mixture was washed using conventional techniques with 0.2 M potassium carbonate three times. The organic layer was dried over magnesium sulfate and evaporated. The resulting mixture was purified by column chromatography on silica gel using 30% methylenechloride in hexane to give pure methyl 7-hydroxycarbonyl-2,4,9-  
20 trithiaadamantane (35-40% yield; melt point  $149^{\circ}\text{C}$  -  $151^{\circ}\text{C}$ ).

### *7-hydroxymethyl-2,4,9-trithiaadamantane*

A flame-dried, 25 mL round-bottomed flask equipped with a Teflon-coated magnetic bar and a septum with an argon inlet was charged with 270 mg (1.10 mmol) of  
25 2,4,9-Trithia-tricyclo[3.3.1.1<sup>3,7</sup>]decane-7-carboxylic acid methyl ester and 5 mL of dry toluene. Cooled by an ice bath, the solution was charged with 1.60 mL of 1.5 M (2.3 mmol) diisobutyl aluminum hydride in hexane. The solution was stirred at  $0^{\circ}\text{C}$  until the complete consumption of the starting material was observed (monitored by TLC). The solution was quenched by 2 mL of methanol and allowed to warm to the ambient temperature. The  
30 filtration through a celite filter cake gave 240 mg (97%) of 7-hydroxymethyl-2,4,9-trithiaadamantane.

***7-carbonyl-2,4,9-trithiaadamantane***

To an acetone-ice cooled three-necked, 25 mL, round bottomed flask equipped with a dropping funnel, was charged with 0.07 mL of oxalyl chloride (0.83 mmol) dissolved in 3 ml of dichloromethane. Dimethyl sulfoxide ( 0.12 mL, 1.66 mmol) was charged into a dropping funnel and added dropwise to a stirred solution of oxalyl chloride. The solution mixture was stirred at  $-78^{\circ}\text{C}$  for 5 minutes. 7-hydroxymethyl-2,4,9-trithiaadamantane dissolved in 5 mL of dichloromethane and a small amount of dimethyl sulfoxide was charged into a dropping funnel and added dropwise to a solution mixture of dimethyl sulfoxide and oxalyl chloride. The reaction was stirred at  $-78^{\circ}\text{C}$  for 45 minutes (reaction monitored by TLC). Triethylamine (5 mL) was added to a stirred solution. The solution was allowed to warm up to the room temperature. Water (20mL) was added to a solution and the mixture was extracted with 10 mL dichloromethane three times. The product was quickly used for the next synthesis because of its poor stability.

***7-ethynyl-2,4,9-trithiaadamantane***

To an ice-cooled solution of sodium hydride in dry toluene, (2-oxo-propyl)-phosphonic acid dimethyl ester was added slowly. The solution mixture was stirred for 1 hour. Methanesulfonyl azide, prepared by the reaction of methanesulfonyl chloride and sodium azide, dissolved in dry toluene and dry tetrahydrofuran was added to a solution. The mixture was allowed to slowly warm up to the ambient temperature and stirred for additional 2 hours. Filtration through a celite filter cake gave yellowish oil of (1-Diazo-2-oxo-propyl)-phosphonic acid dimethyl ester, which was used for the next step without any further purification.

To a solution of aldehyde in 2 mL of dry methanol and potassium carbonate (2 equivalents) was added a solution of (1-Diazo-2-oxo-propyl)-phosphonic acid dimethyl ester (1.2 equivalents) in dry methanol. The solution was stirred for 12 hours. A 20 mL portion of dichloromethane was added to a solution. The resulting organic solution was washed with apportion of 20 mL of 5% sodium bicarbonate. After the evaporation of the solvent, the crude product was purified by column chromatography to yield 7-ethynyl-2,4,9-trithiaadamantane in 75-80% yield.

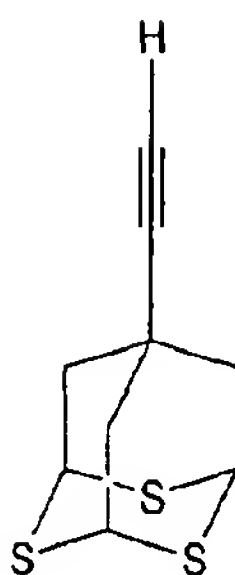
In light of the foregoing, it should be evident that the present invention, which provides: 7-ethynyl-2,4,9-trithiaadamantane, a method for its manufacture, and a method for its use as a tripodal surface anchor substantially improves the art. While, in accordance with the patent statutes, only the preferred embodiments of the present invention have been described in detail hereinabove, the present invention is not to be limited thereto or thereby. Rather, the scope of the invention shall include all modifications and variations that fall within the scope of the attached claims.



## CLAIMS

What is claimed is:

1. A compound having the formula:



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2. A method for manufacturing 7-ethynyl-2,4,9-trithiaadamantane comprising the step of:

reacting 7-carbonyl-2,4,9-trithiaadamantane with Ohira-Bestmann reagent to produce 7-ethynyl-2,4,9-trithiaadamantane.

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3. The method of claim 2, wherein said step of reducing the alkyl 2,4,9-trithiaadamantane-7-carboxylate is performed by reacting the alkyl 2,4,9-trithiaadamantane-7-carboxylate with diisobutylaluminum hydride, sodium tetrahydridoborate, lithium aluminum hydride, or a combination thereof.

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4. The method of claim 3, wherein diisobutylaluminum hydride, sodium tetrahydridoborate, lithium aluminum hydride, or a combination thereof is reacted with the alkyl 2,4,9-trithiaadamantane-7-carboxylate in a relative mole ratio ranging from about 1:1 to about 5:1.

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5. The method of claim 2, wherein the alkyl 2,4,9-trithiaadamantane-7-carboxylate is methyl 2,4,9-trithiaadamantane-7-carboxylate.

6. The method of claim 2, wherein the step of oxidizing 7-hydroxymethyl-2,4,9-trithiaadamantane is performed under Swern oxidation conditions.

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7. The method of claim 2, wherein the Ohira-Bestmann reagent is a combination of X and Y;

wherein X is  $\text{COCH}_3\text{C}(\text{N}_2)\text{P}(\text{O})(\text{OCH}_3)_2$ ,  $\text{COCH}_3\text{C}(\text{N}_2)\text{P}(\text{O})(\text{OCH}_2\text{CH}_3)_2$ , or

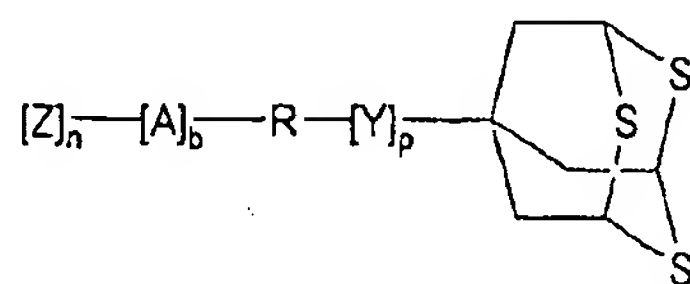
a combination thereof; and

wherein Y is  $\text{K}_2\text{CO}_3$ ,  $\text{Na}_2\text{CO}_3$ , or a combination thereof.

8. The method of claim 2, wherein the Ohira-Bestmann reagent is reacted with 7-carbonyl-2,4,9-trithiaadamantane in a relative mole ratio ranging from about 1:1 to about 5:1.

9. The method of claim 6, wherein the Swern oxidation conditions comprise a mixture selected from the group consisting of a mixture having oxalyl chloride and dimethyl sulfoxide; a mixture having trifluoroacetic anhydride and dimethylsulfoxide; a mixture having triethylamine and diisopropylamine; and combinations thereof.

10. A molecular wire having the formula:



wherein A and Y are independently selected chemical functionalities,

wherein p is 0 or 1,

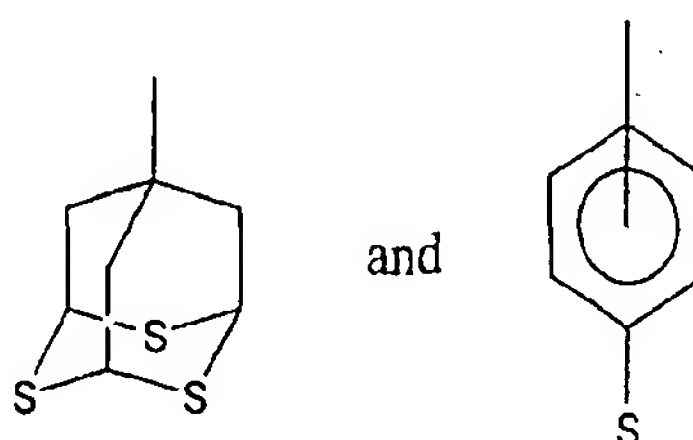
wherein b is 0 or an integer greater than or equal to 1,

wherein R is a compound that is capable of transferring a signal,

wherein Z is a surface anchor, and

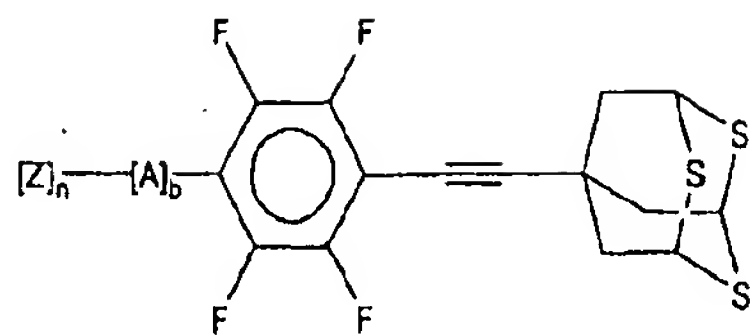
wherein n is 0 or an integer greater than or equal to 1.

11. The molecular wire of claim 10, wherein Z is selected from the group consisting of:

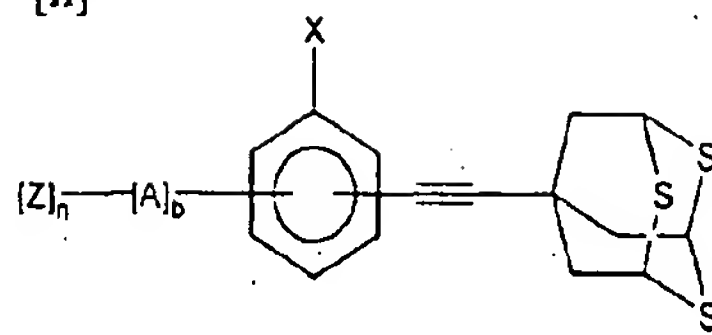


12. The molecular wire of claim 10 wherein A and Y are independently selected from the group consisting of ethynyl and carboxylate.
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13. The molecular wire of claim 10, wherein the wire is selected from the group consisting of:

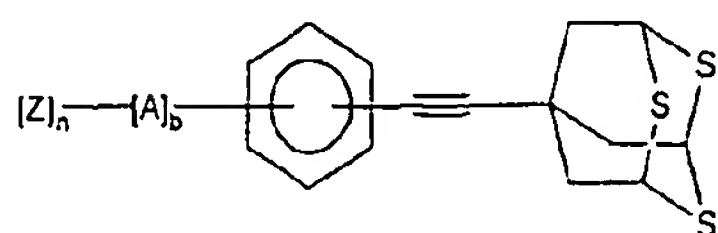
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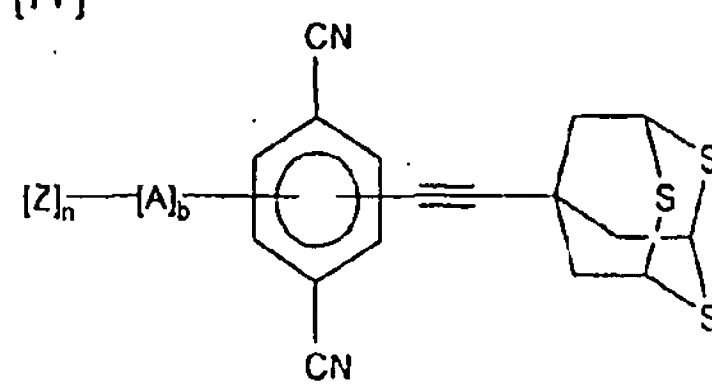
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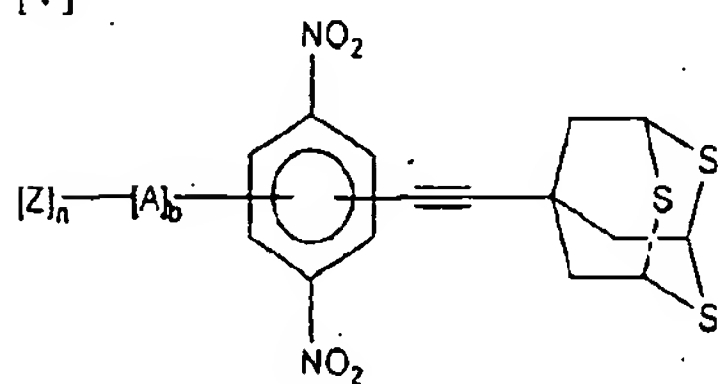
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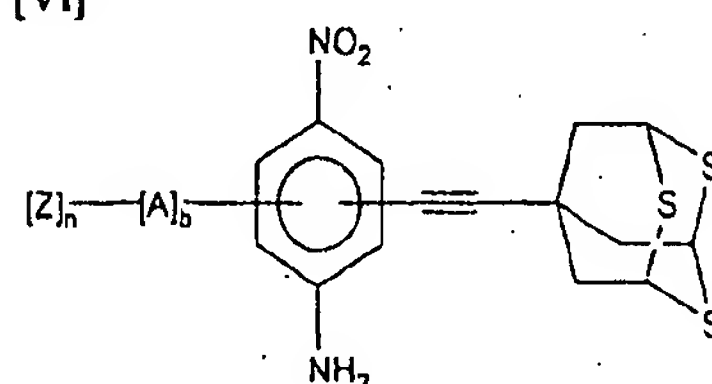
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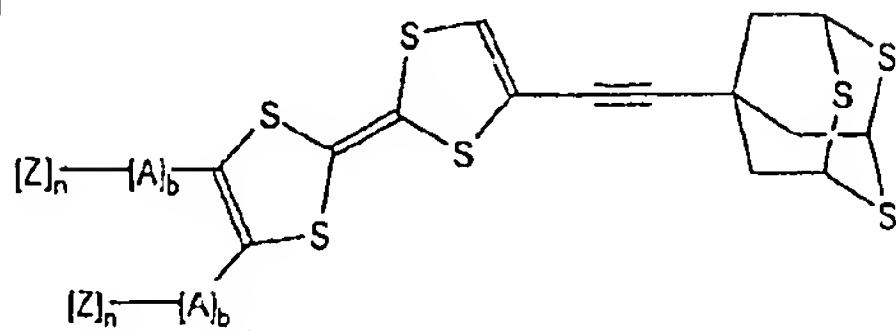
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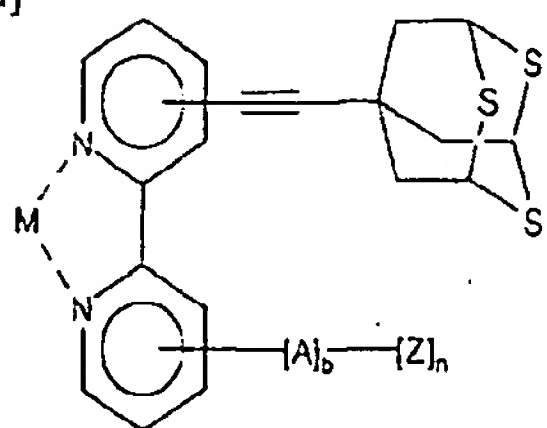
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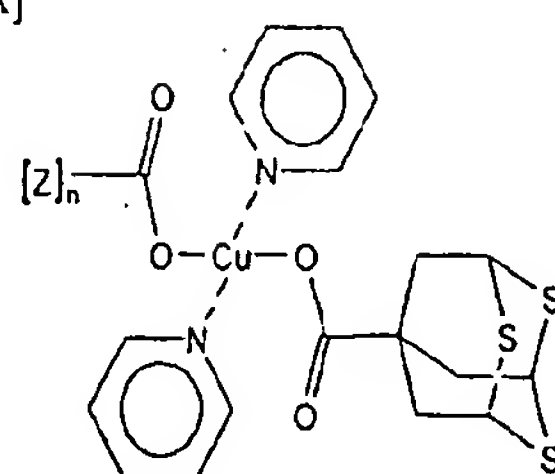
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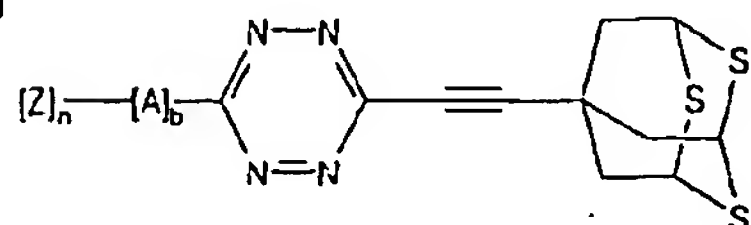
[VIII]



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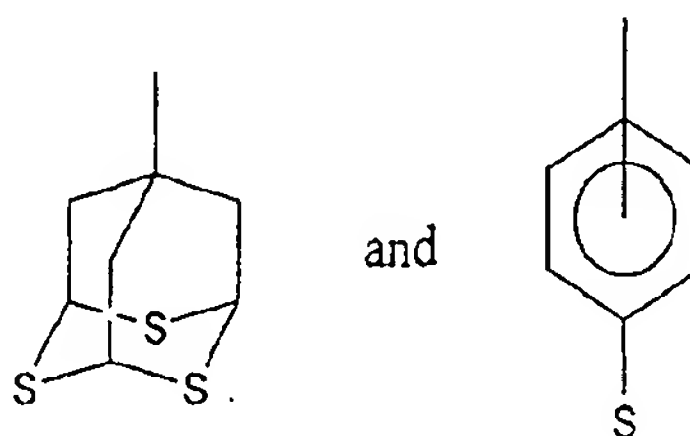
[X]





wherein A is a chemical functionality,  
wherein b is 0 or an integer greater than or equal to 1,  
wherein Z is a surface anchor, and  
wherein n is 0 or an integer greater than or equal to 1,  
wherein M is a metallic element, and  
wherein X is a halogen.

14. The molecular wire of claim 13, wherein M is selected from the group consisting of platinum, palladium, and copper.
15. The molecular wire of claim 13, wherein X is selected from the group consisting of fluorine, chlorine, bromine, and iodine.
16. The molecular wire of claim 13, wherein Z is selected from the group consisting of:



17. The molecular wire of claim 13, wherein A is ethynyl or ester.
18. A method for manufacturing a molecular wire comprising the step of chemically bonding, either directly or indirectly, trithiaadamantane to a compound that is capable of transferring a signal.
19. The method of claim 18, wherein the signal is electronic.
20. A molecular wire produced by the method of claim 18.

21. A method for manufacturing 7-ethynyl-2,4,9-trithiaadamantane comprising the step of:

5           reducing an alkyl 2,4,9-trithiaadamantane-7-carboxylate to produce 7-hydroxymethyl-2,4,9-trithiaadamantane; and

          oxidizing 7-hydroxymethyl-2,4,9-trithiaadamantane to produce 7-carbonyl-2,4,9-trithiaadamantane.

**ABSTRACT OF THE DISCLOSURE**

7-ethynyl-2,4,9-trithiaadamantane and related methods are presented. Manufacturing  
5 7-ethynyl-2,4,9-trithiaadamantane includes the steps of: (1) reducing alkyl 2,4,9-  
trithiaadamantane-7-carboxylate to produce 7-hydroxymethyl-2,4,9-trithiaadamantane; (2)  
oxidizing 7-hydroxymethyl-2,4,9-trithiaadamantane to produces 7-carbonyl-2,4,9-  
trithiaadamantane; and (3) reacting 7-carbonyl-2,4,9-trithiaadamantane with Ohira-  
Bestmann reagent to produces 7-ethynyl-2,4,9-trithiaadamantane.

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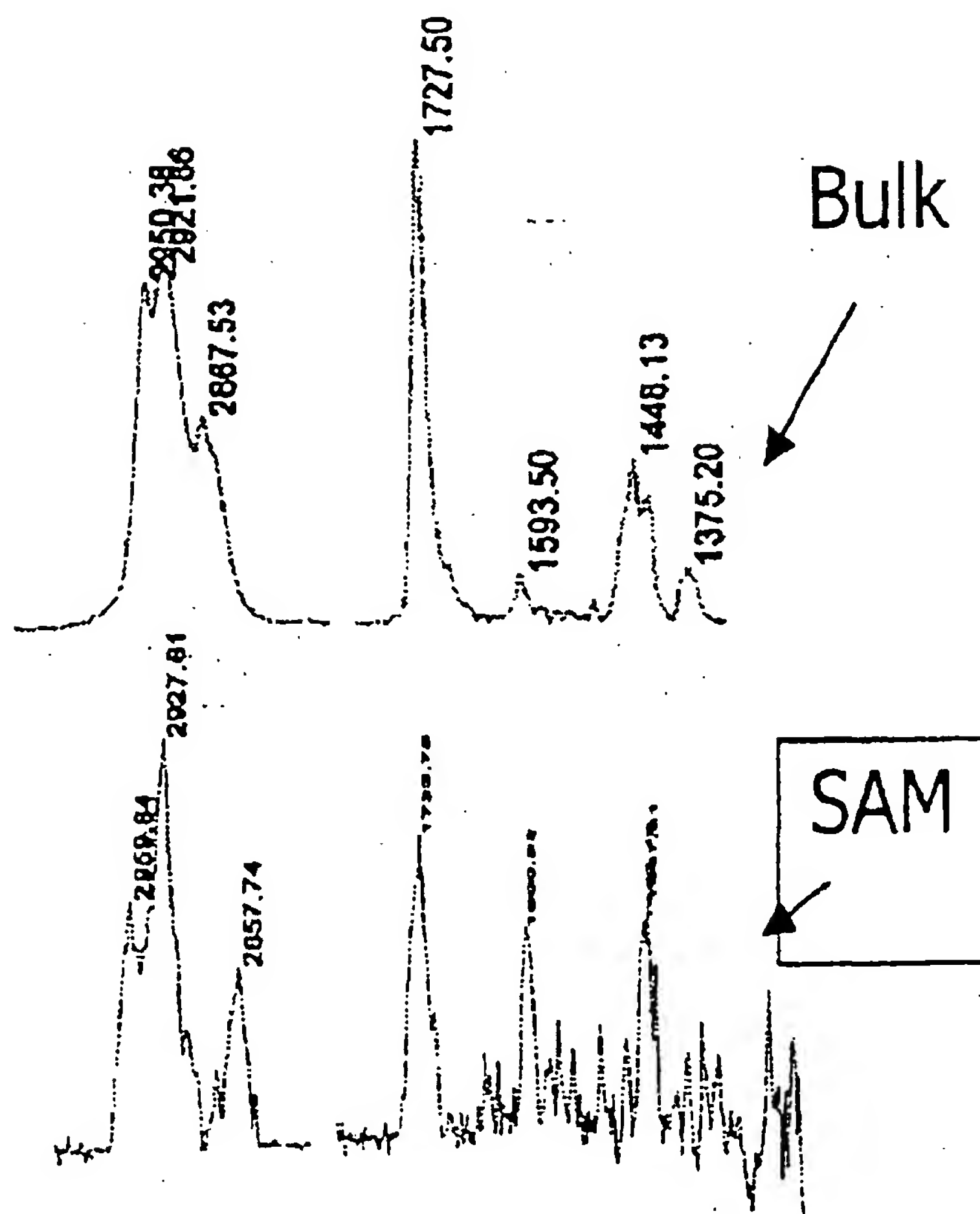


FIG. 1

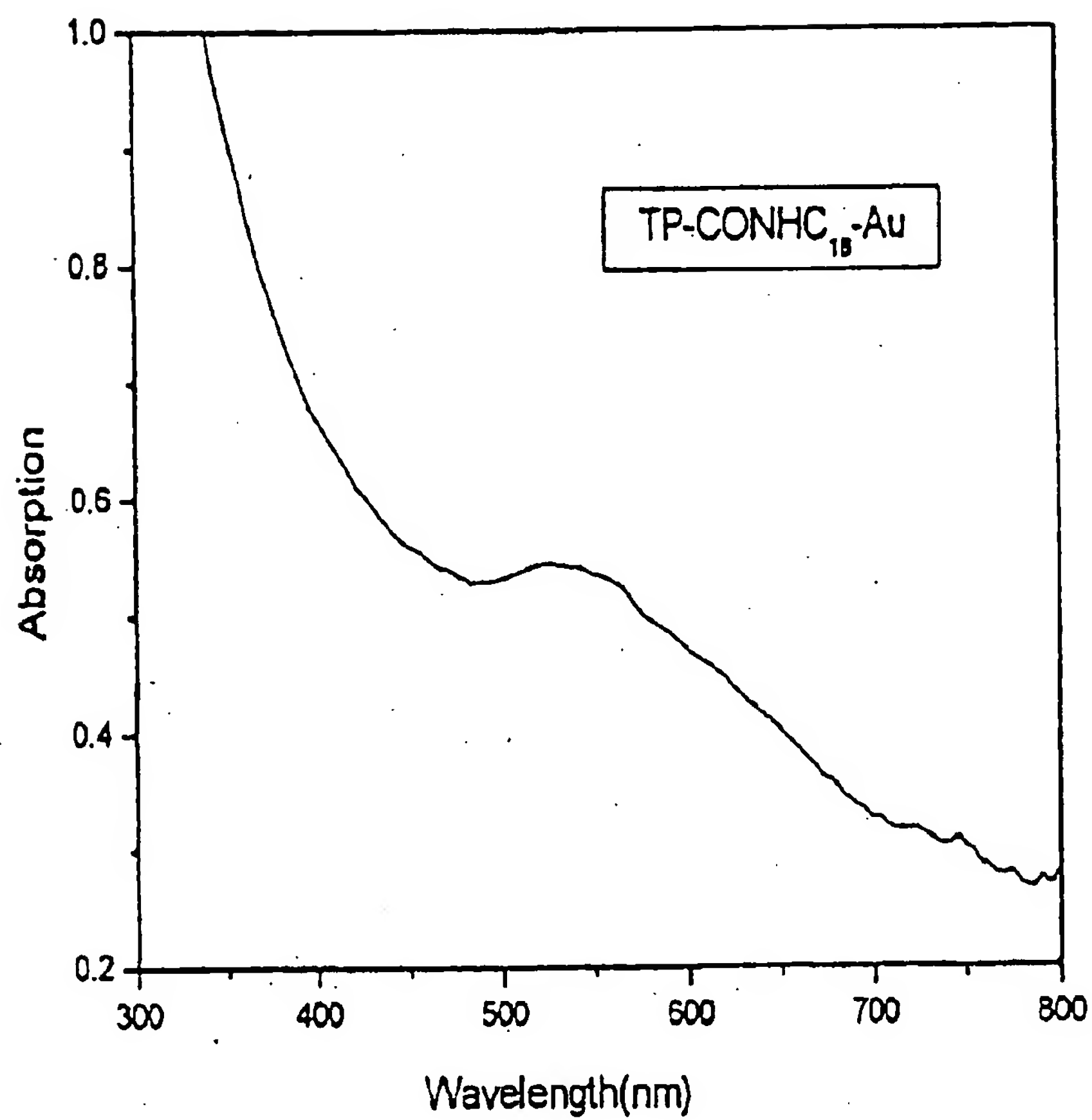


FIG. 2

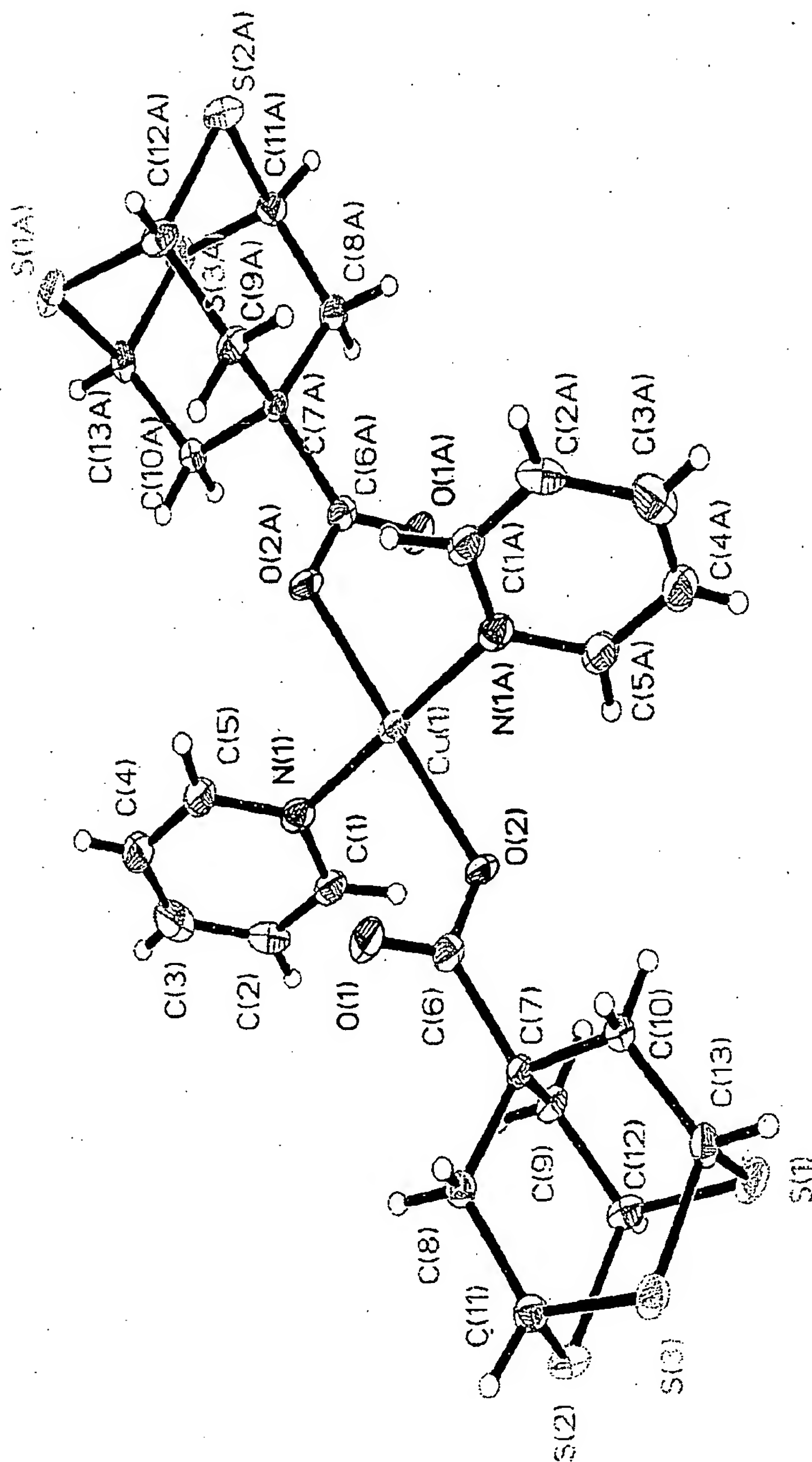


FIG. 3



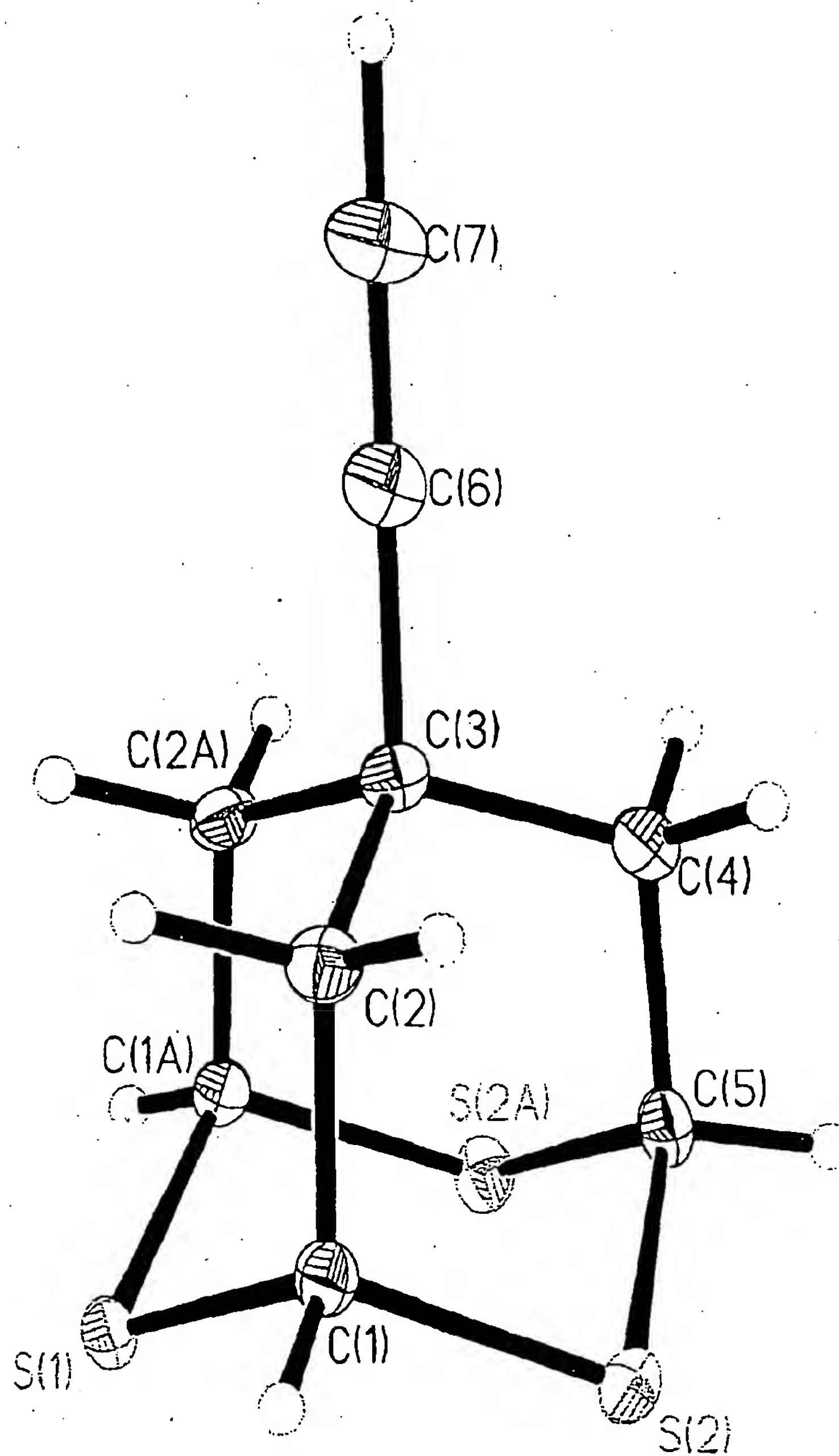


FIG. 4